

Supplementary Information

Ultra-high Density Mechanical Energy Storage with Carbon Nanothread Bundle

Zhan *et al.*

Supplementary Figures

- **Figure 1** | Torsional deformation of an individual nanothread-C under clockwise (CW) and anti-clockwise (ACW) torsion.
- **Figure 2** | Torsional deformation of an individual CNT(10,10).
- **Figure 3** | Bending deformation of an individual CNT(10,10).
- **Figure 4** | Compression of nanothread and CNT triangular lattice under radial compression.
- **Figure 5** | Comparison of nanothread and CNT bundle-7 under relaxation.
- **Figure 6** | Twist deformation of nanothread-A bundle-7 with different sample lengths.
- **Figure 7** | Schematic cross-sectional view of nanothread bundles with different number of filaments.
- **Figure 8** | Different strain components as a function of the torsional strain.
- **Figure 9** | Theoretical failure mode of nanothread and CNT bundles.
- **Figure 10** | Comparison of the normalized gravimetric energy density of CNT bundle under torsion and pure tension.

Supplementary Note

- **Note 1** | Fracture mechanisms of the bundle structure
- **Note 2** | Theoretical description of the bundle deformation
- **Note 3** | Limitations of the theoretical model

Supplementary Videos

- **Video 1** | Compression and relaxation of nanothread-A triangular lattice: only the central filament is shown, and atoms are coloured according to the axial virial atomic stress in the range of 0 to 100 GPa.
- **Video 2** | Compression and relaxation of nanothread-C triangular lattice: only the central filament is shown, and atoms are coloured according to the axial virial atomic stress in the range of 0 to 110 GPa.
- **Video 3** | Torsional deformation of nanothread-A bundle-19: atoms are coloured according to the axial virial atomic stress in the range of 0 to 80 GPa.
- **Video 4** | Torsional deformation of nanothread-C bundle-19: atoms are coloured according to the axial virial atomic stress in the range of 0 to 80 GPa.
- **Video 5** | Torsional deformation of CNT bundle-19: atoms are coloured according to the Von Mises stress in the range of 0 to 60 GPa.